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Title

Crossover form fractal advance to compact advance: Predictions, modeling and experiment

Photonic-bandgap-fiber sensors for gas detection

Adaptive PID Control

Oil shale: A retrospective look. 1. Technologies for extraction & oil recovery

A novel CO₂ capture process integrating amine-based scrubbing with chemical regeneration of spent amine and thermal regeneration of a phase-separation reagent

Numerical Studies of Thermal Stimulation Effects on Methane Production Induced by Depressurization in a Reactor Containing Hydrate-Bearing Porous Media

A 2000 year varve-based climate record from the central Brooks Range, Alaska

Effect of electrical current on SOFC metallic interconnect oxidation in syngas

Effect of H₂S on the performance of Pd4Pt alloy membranes

National Risk Assessment Program: Protecting Groundwater Resources

NETL Extreme Drilling Laboratory Studies High Pressure High Temperature Drilling Phenomena

Parametric Study of Solid Amine Sorbents for the Capture of Carbon Dioxide

Molecular dynamics simulations of methane hydrate decomposition

Stability analysis of doped materials for reversible hydrogen storage in destabilized metal hydrides

Design and Evaluation of Non-fluorous CO₂-Soluble Polymers

Influence of Tert-Amine Groups on the Solubility of Polymers in CO₂

Enhancement of Adsorption Inside Single Walled Carbon Nanotubes--Li Doping Effect on n-Heptane van der Waals Bonding

Atomically-detailed models of gas mixture diffusion through CuBTC membranes

Assessing nanoparticle size effects on metal hydride thermodynamics using the Wulff construction

Influence of Surface Reactions on Complex Hydride Reversibility

Vibron hopping and bond anharmonicity in hot dense hydrogen

The importance of charge-quadrupole interactions for H₂ adsorption and diffusion in CuBTC

Progress, Opportunities, and Challenges for Applying Atomically Detailed Modeling to Molecular Adsorption and Transport in Metal-Organic Framework Materials

Testing the Accuracy of Correlations for Multicomponent Mass Transport of Adsorbed Gases in Metal-Organic Frameworks

Large-scale screening of metal hydride mixtures for high-capacity hydrogen storage from first-principles calculations

DFT characterization of adsorption and diffusion mechanisms of H, As, S, and Se; on the zinc orthotitanate(010) surface

Thermal Conductivity of Methane Hydrate from Experiment and Molecular Simulation

Identification of Destabilized Metal Hydrides for Hydrogen Storage Using First Principles; Calculations

Selective growth of Fe₂O₃ nanoparticles and islands on Au (111)

Hydrogen production from coal/biomass and waste gas via sorption-enhanced WGS reaction and catalytic decomposition of hydrogen sulfide

Heat transfer for alternative fuels and engine cycles

Hydrogen Sulfide and Carbon Dioxide Removal from Fuel Gas Streams Using and Ionic Liquid as a Physical Solvent

Modeling, Identification, and Control of a Cold Flow Circulating Fluidized Bed: A Thesis

First Principle Analysis of the Interaction of Carbon Dioxide with Functionalized Tertiary Amidines

Modeling of particle trajectories of coal size and density fractions in a gasifier: A Thesis

Ab initio Calculations to Determine the Optimal Conditions for a Given CO₂ Capture Sorbent

The interaction of spherical Al₂O₃ particles with molten Al₂O₃-CaO-FeOx-SiO₂ slags

Scalar filtered density function for large eddy simulation of a bunsen burner

Carbon Capture Possibilities through Electrochemical Air Separation and Oxy-Fuel Combustion

Numerical simulations examining the relationship between wall roughness and fluid flow on rock fractures

Experimentally measured interfacial area during lateral air injection into a water-saturated porous media

Characterization of Mn-Co Electrodeposition Process by QCM

Photoinduced Electron Paramagnetic Resonance Study of Electron Traps in TiO₂ Crystals: Oxygen Vacancies and Ti³⁺ Ions

Impact of fuel contaminants on performance in coal-based SOFCs

CO₂-Photo-catalytic reduction: Characterization of Fe-doped-TiO₂

Adsorption and Diffusion of Light Gases in ZIF-68 and ZIF-70: A Simulation Study

A lifting methodology for airfoils in hydrogen-fired and oxy-fuel turbines: Creep damage

On the effect of sub-grid drag closures

Mn-Co electroplating on SS for SOFC interconnects

First Principles Study of Vacancy and Tungsten Diffusion in fcc Cobalt

Towards the development of graphitic nanocapsules as storage media with toxicity mitigation

Theoretical Screening of Oxides and Hydroxides for CO₂ Sorbents

Elastic and Thermodynamic Properties of Cr-V Binary Alloys Predicted from First Principles Calculations

Technology Transfer Success (2 posters)

Develop novel coatings for SOFC interconnect

Exploratory design study on reactor configurations for carbon dioxide capture from conventional power plants employing regenerable solid sorbents

Modeling CO₂ capture by molecular organic frameworks

Preliminary Evaluation of Coal-and Biomass-derived Chars as Beneficial Soil Amendments

Soil Quality of Landfills Used for Oil Bioremediation in Northwest Pennsylvania

Detection of Lead Mobilization from Soil at an Abandoned Sulfuric Acid Recycling Plant Using Rock Phosphate-Immobilized Gel Beads

Composition Spread Alloy Films for High-Throughput Characterization of PdxCu100-x

Exceptional High-temperature Stability through "Distillative" Self-stabilization in Bimetallic Nanoparticles

The Interface Between Refractory Liners and Molten Slags in Fuel Flexible Gasifiers

Thermodynamic Assessment of CR-Rare Earth Systems

Materials and component development for advanced turbine systems

Aero-thermal modeling and experiments of turbine airfoils

Airfoil life prediction modeling

A load-based depth-sensing indentation technique for NDE and damage assessment of TBC's

Mechanism of Shell Growth on Pt@Fe Nanoparticles

Advanced APS thermal barrier coatings

Photo-electro-catalytic-reduction of CO₂: Catalyst characterization

Develop novel coatings for SOFC interconnect

Minimization of fresh water consumption for pulverized coal (PC) power plants

Nondestructive Evaluation of Thermal Barrier Coatings using Acousto-Ultrasonic Techniques

Lean-burn stationary natural gas engine operation with a prototype laser spark plug (ICES2009-76013)

Fundamental Studies on Controlling Scale Growth in Alloys through Additions of Reactive Elements Over-layer on TBC for increasing TBC thermal insulation

Advanced APS thermal barrier coatings

Development of diffusion barrier coatings for high temperature applications

A Superstructure-based Optimal Synthesis of PSA Cycles for Pre-Combustion CO₂ Capture

Effects of Oxyfuel Atmospheres and Surface Deposits on Alloy Corrosion

A superstructure-based optimal synthesis of PSA cycles for pre-combustion CO₂ capture

North Dakota lignite and Pittsburgh bituminous coal: a comparative analysis in application to CO₂ Sequestration.

Effects of Water-table and Topography on the Near-Surface Migration of Injected CO₂

Velocity measurements in reservoir samples from the SACROC unit using various pore fluids, and integration into a seismic survey taken before and after a CO₂ sequestration flood.

Solubility of CO₂ in CO₂-philic Oligomers; COSMOtherm Predictions and Experimental Results

Characterization of ZnO nanoparticle suspension in water: Effectiveness of ultrasonic dispersion

Nanocomposite Oxygen Carriers for Chemical Looping Combustion of Sulfur Contaminated Synthesis Gas

Mount Elbert Well, A review of coring operations and sediment core lithostratigraphy

Pore fluid geochemistry from the Mount Elbert gas hydrate stratigraphic test well

Comparison of the Properties of Xenon, Methane, and Carbon Dioxide Hydrates from Equilibrium and Nonequilibrium Molecular Dynamics Simulations

Reforming Liquid Hydrocarbons with Ni-substituted Barium Hexaaluminates: Effect of Oxygen-Conducting Support

Nonlinear Fluid Flow Over a Wavy Surface

Development of a Transferable Reactive Force Field for Cobalt

Intrinsic properties of sediment from the BPXA-DOE Mount Elbert gas hydrate research well

Decorated carbon nanotubes with unique oxygen sensitivity

Hydrogen Dissociation on Pd4S Surfaces

Sorption-enhanced water gas shift reaction by novel solid sorbents

Mapping Near-Surface Electromagnetic Properties by Airborne Surveys to Improve Water Management from Gas Production in the Powder River Basin

Radiation modeling in oxy-fuel combustion

Advanced APS Thermal Barrier Coatings

Effects of Carbon Dioxide and Water Vapor on Selective Oxidation of Fe-Cr Base Alloys Relevant to Oxyfuel Combustion

The impact of moisture on the energetics for an amine-based sorbent used for carbon dioxide capture

Proof-of-concept testing with an electrochemical cell for carbon dioxide separation from flue gas

The role of solid oxide fuel cells in advanced hybrid power systems of the future

Origin of photocatalytic activity of nitrogen-doped TiO₂ nanobelts

Mechanism for the Dynamic Adsorption of CO₂ and CH₄ in a Flexible Linear Chain Coordination Polymer as Determined from In-Situ Infrared spectroscopy

Flexible capacitive sensor for circumferential detection of defects in buried natural gas plastic pipelines

The Evolution of Oxide Ridges During Scaling of Fe-22wt%Cr Alloys

Stability of a Class of Discrete Nonlinear Recursive Observers

Ionic liquid membranes for carbon dioxide separation

Shape-enhanced photocatalytic activity of single-crystalline anatase TiO₁ (101) nanobelts

Development of Rock Phosphate-Agarose Gel Beads to Monitor the Release of Lead into Stream Water from a Contaminated Industrial Site

Thermal regime of the Trough Creek Ice Mine, Huntingdon County, Pennsylvania

Synthesis and Characterization of a New One-Dimensional Nanoporous Material: Zn(tbip)

Gas hydrate: Energy potentiality and environmental liability

Robust nonlinear model predictive control based on discrete nonlinear extended observers

Convection-radiation heat transfer in a nonlinear fluid with temperature-dependent viscosity

Use of piezoelectric pressure transducers to determine local solids mass flux in the riser of a cold flow circulating fluidized bed

Post and pre-stack seismic reflection data processing of a 3D reflection seismic survey over a CO₂ injection

Advanced Analysis of SEM and CT SACROC limestone imagery to obtain porosity statistics (pore percentages, sizes, and connectivity) for use in chemical and geophysical modeling

Velocity measurements in reservoir rock samples from the SACROC unit and integration into a 4D seismic survey of a CO₂ sequestration flood

The effects of changing apertures on the transmissivity of rough fractures

Prediction of CO₂ Solubility in Oligomers

A mechanistic study on the reaction of monoethanolamine (MEA) with CO₂ in aqueous solution

Visible light photoreduction of CO₂ using CdSe/Pt/TiO₂ heterostructured catalysts

First Principles Study of Cr-Ti Binary System

Role of lattice oxygen in the partial oxidation of methane over Rh/supported ceria catalysts isotopic studies

Hydrogen production over Ni/ceria supported catalysts by partial oxidation of methane

Fe-doped-TiO₂ characterization: CO₂ photo-catalytic activation

Perovskite Catalyst Design for Electrochemical Oxygen Separation

Conversion of a TEM10 beam into two nearly Gaussian beams

Preparation and characterization of Fe₃O₄ (111) nanoparticles and thin films on Au (111)

Synthesis and Rheological Properties of cation-exchanged Laponite suspensions

Mono-and terfluorene oligomers as versatile sensitizers for the luminescent Eu³⁺ cation.

Biochar, biodiversity and greenroofs: Carbon sequestration and environmental conservation in urban environments

Strontium isotope quantification of deep brine and shallow acidic coal mine drainage inputs to high TDS gas well discharges in western Pennsylvania

Sulfate removal from oil shale retort water and electricity generation using microbial fuel cells: Effects of carbon:sulfate ratio and reactor configuration

Laser spark plug development and engine testing: Design of a diode side pumped solid state passively Q-switched laser for use as an ignition source for a lean-burn stationary natural gas engine

Velocity measurements in reservoir rock samples from the SACROC unit using various pore fluids and integration into seismic survey taken before and after CO₂ sequestration flood

Lean-burn stationary natural gas reciprocating engine operation with a prototype fiber couples diode end pumped passively Q-switched laser spark plug

Radio frequency plasma spark plug development and engine testing: Design of a quarter-wave coaxial cavity resonator for use as an ignition source for an internal combustion engine

Lean-burn stationary natural gas engine operation with a prototype laser spark plug

North Dakota lignite and Pittsburgh bituminous coal: A comparative analysis in application to CO₂ sequestration

Carbon dioxide transport and sorption behavior in confined coal cores for carbon sequestration

Partial oxidation of liquid hydrocarbons in the presence of oxygen-conducting supports for solid oxide fuel cells: Effect of catalyst layer deposition

Derivative-free optimization: A review of algorithms and comparison of software implementations

Comparison of experimental and numerical two-phase flows in a porous micro-model

New title: Two-phase flow in porous media: Predicting its dependency on capillary number and viscosity ratio. Previously titled: Crossover from fractal viscous fingering to compact invasion for drainage: modeling and experiment

Flow simulations for carbon sequestration at a coal-seam pilot site

The role of geology and shallow lithostrigraphy in the distribution of methane flux through shallow sediments across the Beaufort Shelf of Alaska

Accelerating clean and efficient coal gasifier designs with high performance computing

Robust stability of nonlinear model predictive control with extended Kalman filter and target setting

Thin Films of Single-walled Carbon Nanotubes for Flexible Electronic Device Applications

Localization of Frontier Orbitals on Anatase Nanoparticles Impacts Water Adsorption

Where are the active sites of anatase nanoparticles?

Coal-gas Interaction: Implications of changes in texture and porosity

Synthesis-structure-property relationships for hyperbranched aminosilica CO₂ adsorbents

NETL amine-based solid sorbents for capture of CO₂

Designing amine-based solid sorbents for post combustion carbon dioxide capture

Single crystalline La_{0.5}SR_{0.5}MnO₃ microcubes as cathode of solid oxide fuel cell. PREVIOUSLY TITLED
Electrochemical oxygen reduction properties of LSM microcubes

Modeling and Simulation of the Chemical Looping Combustion Reactor

Characterizing the correlations of failure events: A 2-d block and springs model

Catalytic cycloaddition of CO₂ to epoxide over Pt nanoparticles supported on self assembled coordination polymers

Influence of a chelating agent on activity of SiO₂ supported cobalt catalyst for Fischer-Tropsch synthesis

PhoucX., Howard, Bret H., Chyu, Minking K. XST40 Yes Yes

TPR-2740 Preparation and characterization of Fe304 (111) nanoparticles and thin films on Au (111) Deng, X.; Lee, J.; Matranga, C. 660 - Chemistry Surfaces Science No No Yes Yes Physical Chemistry Chemical Physics published by Royal Society of Chemistry Materials Science

TPR-2739 In-situ impedance measurements of LiMn1.5Ni0.4Cr0.1O4 cathode during charge/discharge cycling Asmar, K.; Singhal, R. ; Katiyar, R.; Sakla, A.; Abernathy, H.; Manivannan, A. 620 - Energy Systems Dynamics Yes Yes Materials Challenges in Alternative & Renewable Energy 2010, Cocoa Beach, FL, February 21-25, 2010 02/21/2010 Energy System Dynamics

TPR-2738 Conversion of a TEM10 beam into two nearly Gaussian beams Buric, M.P.; Falk, J.; Woodruff S.D. 606 - University Collaboratory No No Yes No Applied Optics, 49 (2010) 739-744 Energy System Dynamics 02/01/2010

TPR-2737 Infrared Spectroscopic Adsorption Studies - Carbon Capture and Storage Chirdon, D.; Culp, J.; Goodman, A. 660 - Chemistry Surfaces Science Yes No No No 2009 Symposium at the University of Pittsburgh, October 15 and 16, 2009 10/15/2009 Materials Science

TPR-2736 Perovskite Catalyst Design for Electrochemical Oxygen Separation Landon, J.; Kitchin, J. 600 - University Collaboratory No Yes No No Pittsburgh Coal Conference, Sept. 22-23, 2009, Pittsburgh, PA 09/22/2009 Energy System Dynamics

TPR-2735 Fe-doped-TiO2 characterization: CO2 photo-catalytic activation Salazar, M.; Miller, A. 610 - Separations Fuels Processing Yes Yes International Journal of Oil, Gas and Coal Technology Energy System Dynamics

TPR-2734 Hydrogen production over Ni/ceria supported catalysts by partial oxidation of methane Salazar, M.; Reyes, B. 610 - Separations Fuels Processing Yes Yes International Journal of Hydrogen Energy Energy System Dynamics

Integrating velocity measurements in a reservoir rock sample from the SACROC unit with an AVO proxy for subsurface supercritical CO2

Particle clusters in and above fluidized beds

Constraints on methane distribution from acoustic profiles of shallow sediments across the Alaska shelf Subseafloor macroscopic biofilms involved in anaerobic oxidization of methane

The role of geology and shallow lithostratigraphy in the distribution of methane flux through shallow sediments across the Beaufort Shelf of Alaska

Preliminary geochemical survey of shallow sediment methane flux across the Alaskan Beaufort Sea shelf

Lithostratigraphic analysis and sedimentology of cores from the Mount Elbert-01 gas hydrate stratigraphic well

Lithostratigraphic analysis of sand and silt facies from NGHP 01 gas hydrate accumulations in the Krishna-Godavari Basin

Understanding Sensor Response of metal Decorated Carbon Nanotubes

Transient Oxidation and Grain Boundary Characteristics

Ideal and Defect interstitial Channel Availability in Carbon Nanotube Bundles: Comparison of Modeling with Experiments

High resolution simulations of coal jets in a gasifier
Au-mixed lanthanum/cerium oxide catalysts for water-gas-shift

Experimental and CFD analysis of bubble parameters in a variable thickness fluidized bed

Mathematical modeling and numerical simulation of methane production in a hydrate reservoir
A comparative study of eight finite-rate chemistry kinetics for CO/H₂ combustion

Simulation of a swirling gas-particle flow using different k --- e Models and particle-parcel relationships
Unsteady motion of a non-linear viscoelastic fluid

Separation of CO₂ from flue gas using electrochemical cells

Surface characterization of palladium-alumina sorbents for high-temperature capture of mercury and arsenic from fuel gas

Environmental effects of natural gas production from the Marcellus Shale

Estimate of solid flow rate from pressure measurement in circulating fluidized bed

Near-surface monitoring for the ZERT shallow CO₂ injection project

Electrochemical reduction of CO₂ in KHCO₃ aqueous solution

A voltammetric study of reduction of CO₂; Effect of type of solvent

Electrochemical Concentration of Carbon Dioxide from an Oxygen/Carbon Dioxide Containing Gas Stream

Organization

650 - Geosciences

620 - Energy Systems Dynamics

670 - Computational Science

670 - Computational Science

650 - Geosciences

660 - Chemistry Surfaces Science

640 - Environmental Science

606 - University Collaboratory

660 - Chemistry Surfaces Science

650 - Geosciences

630 - Engineering Research; 605 - Earth and Mineral Sciences

610 - Separations Fuels Processing

605 - Earth and Mineral Sciences

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600 - Office of Research & Development

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660 - Chemistry Surfaces Science

690 - Process Development

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Focus Area

Energy System Dynamics
Computational & Basic Science
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